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THE CALCULATION OF LINE WIDTHS

~~Work done~~ by:
M. Baranger
J. C. Stewart

Report written by:
M. Baranger

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THE CALCULATION OF LINE WIDTHS

Causes of line width

1. Doppler effect. The theory of it is simple enough.

2. Natural width. Again the theory is well-known and easy to apply, and one can check that this cause of width is not important compared to the following two.

3. Width due to electrons in the plasma. This is the main subject of this report.

4. Width due to the ions. This will be briefly discussed at the end.

The electron width

We pick as an example the case of the $2p \rightarrow 3d$ line in C_{IV}, which is one of the most important lines in the CH_2 opacity. Typical conditions are $kT = 10$ volts and $\Gamma = 2000$, which give an electron density $n_o = 9.5 \times 10^{19} cm^{-3}$ (from Bernstein and Dyson, GAMD-865). The impact approximation (Phys. Rev. 111, 494; 112, 855) is very good in this case, i.e., the effect of the electrons is to give the line a Lorentz shape

$$I(\omega) \sim \frac{1}{(\omega - \omega_o - d)^2 + w^2}$$

with a shift d (which turns out to be small) and a width w. One may ask how far down in the wings the line will keep its Lorentz shape. The usual answer, for an isolated line, is out to a distance from the line center of order τ^{-1}, where τ is a typical collision time. In our case, τ^{-1} turns out to be roughly 4 volts. However, rather close to the $2p \rightarrow 3d$ line, namely .6 volt away, there is the forbidden line $2p \rightarrow 3p$. Our isolated-line shape cannot go on past this point. Beyond .6 volt, one would have to use the theory of overlapping lines. This would be roughly equivalent to computing a new line width, again by the impact approximation, but assuming the 3d and 3p levels to be degenerate. This might work fairly well on the high-frequency side of the line, which is the side opposite to the forbidden line. We shall not do it here, but shall just compute the width of the central core. Note also that, 2.7 volts away from the line, we would run into the $2p \rightarrow 3s$ line, which however is weak.

Both the lower, 2p level and the higher, 3d level are affected by the electrons. But, for a first estimate of the width, we may neglect their interaction with the 2p level, which is tighter than the other. This has the advantage of simplifying the s[illegible] over magnetic quantum numbers considerably. Then the width is si[illegible]y given by

$$\nu = \frac{1}{2} n_o v \sigma$$

where σ is the total cross-section for scattering an electron by the ion in the 3d state, averaged over the magnetic quantum number. We should also average over the Maxwell distribution for the electron velocity v.

Calculation of the cross-section

If we assume C_{IV} to be formed of a central core of charge $4e$ surrounded by a single looser electron, the interaction between the perturbing electron and the ion has the form

$$-\frac{4e^2}{r_2} + \frac{e^2}{r_{12}} \qquad \left(\begin{array}{ll} r_2 : & \text{perturbing electron} \\ r_1 : & \text{bound electron in ion} \end{array} \right)$$

One may try to use perturbation theory, using

$$H_o = H_{ion} + \frac{p_2^{\,2}}{2m} - \frac{3e^2}{r_2}$$

as the unperturbed Hamiltonian and

$$H_1 = \frac{e^2}{r_{12}} - \frac{e^2}{r_2}$$

as the perturbation. Simple estimates show that 1st order perturbation theory will probably be pretty good, except perhaps for the very lowest ℓ_2 values of the perturbing electron, so we adopt it. It is furthermore clear that the dipole part of H_1 makes the biggest contribution, so we consider it alone for the beginning. In first order, it can give rise only to inelastic collisions, since both ℓ_1 and ℓ_2 must change by one unit. Finally, since r_2 is usually bigger than r_1, we write the dipole part of H_1 as if this were

always so, namely

$$H_1 = \frac{4\pi e^2}{3} \frac{r_1}{r_2^{\,2}} \sum_M Y^*_{1M}(\Omega_1)\, Y_{1M}(\Omega_2) .$$

Of the three approximations we just made, the one involving keeping only the dipole is the easiest to correct, by actually looking at other multipoles. The one involving the use of 1st order perturbation theory may be improved by looking at the 2d order contribution to the elastic scattering (this was found to be very small for the present line) and by cutting off the sum over ℓ_2 where 1st order perturbation theory stops being valid, saying that, for smaller values of ℓ_2, every collision interrupts the radiation completely (this correction was also rather small). The 3d approximation, assuming $r_2 > r_1$, is the hardest one to get away from and its validity may still be open to question.

If these three approximations are made, the problem becomes identical with that of the Coulomb excitation of nuclei, and all relevant formulae may be looked up in the review article by Alder et al in Revs. Mod. Phys. 28, 432 (1956). It is also good to remember that, since the number of values of ℓ_2 that contribute is large (λ_2 is of order 5×10^{-9} cm), the classical approximation is quite good for most purposes, i.e., one can think of the electrons as moving on hyperbolic trajectories and perturbing the ion through their time-dependent electric field.

Results

We use Eqs. (II B.37), II A.18), (II A.16), (IIA.13) of Alder and the result can be written in the form

$$\nu = \frac{4\pi}{3} n_o v k^2 \sum_f \frac{\max(\ell_1, \ell_f)}{2\ell_1 + 1} \left(\frac{R_{fi}}{a_o}\right)^2 \frac{9}{32\pi^2} f_{E1}(\eta_1, \xi)$$

The sum is over all final states of the ion to which dipole transitions are possible, but in practice only states in the same shell as the initial one (in our example, only the 3p state) are of any importance. (R_{fi}/a_o) is the radial matrix element of r

$$R_{fi} = \int_0^\infty R_i(r)\, R_f(r)\, r^3 dr$$

in units of the Bohr radius. For this one can use the hydrogenic value (Bethe and Salpeter, Eq. 63.5) divided by Z (4 in our case) or the better value of Bates and Damgaard. We have

$$\eta_1 = \frac{Z'e^2}{\hbar v_1} \quad (Z' = 3 \text{ for our example})$$

$$\eta_2 = \frac{Z'e^2}{\hbar v_2}$$

$$\zeta = \eta_2 - \eta_1$$

When the excitation energy ΔE is small compared to the energy of the electrons E, we have

$$\zeta = \eta \frac{\Delta E}{2E} .$$

f_{EI} is tabulated in various places, in particular Alder et al. However, these authors are concerned about the repulsive Coulomb case, while we have the attractive case. The connection between the two is

$$f_{EI\ \text{attractive}} = e^{2\pi\zeta} f_{EI\ \text{repulsive}},$$

which follows from Eq. (II B.59) of Alder.

We have yet to perform the average over the Maxwell distribution. Since f_{EI} is a rather slow function of E, and since the other factors in v are proportional to $\frac{1}{v}$, one should use for the velocity the inverse of the average of $\frac{1}{v}$, which is

$$v_o = \left(\frac{8}{\pi}\frac{kT}{m}\right)^{1/2}$$

The corresponding energy is

$$E_o = \frac{1}{2} m v_o^2 = \frac{4}{\pi} kT .$$

For a more accurate evaluation of this average, one can use the work of J. M. Berger, Ap. J. 124, 550 (1956).

For our example, $\zeta = .15$, $\eta = 4$, and we can use the classical limit of f_{EI}. We find from Alder et al.

$$\frac{9}{32\pi^2} f_{EI\ \text{attractive}}(\zeta) = 2.93 .$$

It is interesting to compare this with what we would have obtained, had we forgotten about the Coulomb potential, $-3e^2/r_2$, between the perturber and the origin, which classically amounts to assuming straight line trajectories. The result in this case is given by Alder's Eq. (II E.24) (the Born approximation result) and is

$$\frac{9}{32\pi^2} f_{EI} = \ln \frac{\eta_1 + \eta_2}{\eta_2 - \eta_1} = \ln \frac{4E}{\Delta E} = 3.97 .$$

We reach the paradoxical conclusion that the Coulomb corrections actually decrease the width, instead of increasing it. The reason for this can be found in the fact that, for $\ell_2 > \eta$, the trajectory is still almost a straight line, and the Coulomb correction is not important, while for $\ell_2 < \eta$, the hyperbola doubles upon itself, the axial component of the electric field of the perturber changes sign twice during the collision, and this makes it less efficient in first order. It is true that, for a given ℓ_2, the hyperbola comes closer to the ion than the straight path, but this is compensated by the fact that the electron on the hyperbola is moving faster and has less time to act.

The Debye length cut-off

When ΔE decreases, the width increases logarithmically. This divergence can be traced to the large impact parameters, and should actually be cut-off when the impact parameter reaches the Debye length, because the electric field is then shielded by the other electrons. This amounts to replacing ΔE in the logarithm by $\hbar\omega_p$ where ω_p is the plasma frequency

$$\omega_p = \left(\frac{4\pi n_o e^2}{m}\right)^{1/2} .$$

The electronic width of the 3p ⟶ 3d line in C_{IV}

After inclusion of the bound state correction, the width turns out to be .0185 volt, a very small number. On the other hand, if we had assumed straight trajectories (or Born approximation) and no bound states, we would have obtained a slightly larger width, namely .021 volt, a very surprising result!

Width due to the ions

In contradistinction to the electrons, the ions may be treated by the adiabatic approximation since they move much more slowly. For a given configuration of the ions, the interaction energy and the wave function may be calculated by Stark effect theory. However, the static theory is not necessarily valid. The criterion for its validity is $\tau\omega \gg 1$, where τ is a typical collision time and ω the static width. In our example, the number $\tau\omega$ was found to be appreciably smaller than one, which means that the impact approximation again is valid. Here however, the elastic collisions are the ones that contribute and the Stark interaction energy should be used as the perturbation. The ion width was found to be only a fraction of the electron width (but there is a sizeable ion shift). This may not be the case for all lines: at higher quantum numbers, the Stark effect becomes stronger and more nearly linear, the static theory becomes valid, and the ions play a vital role in determining the shape of the line and whether or not it overlaps with its neighbors.

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END